



chain nodes :  
 22 23 24 25 26 27 49 50 51

ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 28 29 30 31 32  
 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48

chain bonds :  
 5-16 19-22 22-23 23-24 24-25 25-26 26-27 32-43 46-49 49-50 50-51

ring bonds :  
 1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 6-12 7-15 8-9 9-10 10-11 12-13 13-14 14-15  
 16-17 16-21 17-18 18-19 19-20 20-21 28-29 28-34 29-30 29-35 30-31 30-38 31-32  
 32-33 33-34 33-39 34-42 35-36 36-37 37-38 39-40 40-41 41-42 43-44 43-48 44-45  
 45-46 46-47 47-48

exact/norm bonds :  
 1-2 1-7 3-4 4-5 5-6 5-16 16-17 16-21 17-18 18-19 19-20 19-22 20-21 23-24 24-25  
 26-27 28-29 28-34 30-31 31-32 32-33 32-43 43-44 43-48 44-45 45-46 46-47 46-49  
 47-48 50-51

exact bonds :  
 22-23 25-26 49-50

normalized bonds :  
 2-3 2-8 3-11 6-7 6-12 7-15 8-9 9-10 10-11 12-13 13-14 14-15 29-30 29-35 30-38  
 33-34 33-39 34-42 35-36 36-37 37-38 39-40 40-41 41-42

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom 31:Atom  
 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom  
 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS

fragments assigned product role:  
 containing 1

fragments assigned reactant/reagent role:  
 containing 28

